

REPORT DOCUMENTATION PAGE

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MEMORANDUM FOR PR (In-House Publication)

FROM: PROI (TI) (STINFO)

18 May 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-TP-2000-117**
Perkins, Dr. Leslie, "Computational Chemistry and Materials Science CTA"

High Performance Computing Mod. Office
(no location given, 27 Mar 00)

(Statement A)
(Submission Deadline: N/A)

1. This request has been reviewed by the Foreign Disclosure Office for: a.) appropriateness of distribution statement, b.) military/national critical technology, c.) export controls or distribution restrictions, d.) appropriateness for release to a foreign nation, and e.) technical sensitivity and/or economic sensitivity.

Comments: _____

Signature _____ Date _____

2. This request has been reviewed by the Public Affairs Office for: a.) appropriateness for public release and/or b) possible higher headquarters review.

Comments: _____

Signature _____ Date _____

3. This request has been reviewed by the STINFO for: a.) changes if approved as amended, b.) appropriateness of distribution statement, c.) military/national critical technology, d.) economic sensitivity, e.) parallel review completed if required, and f.) format and completion of meeting clearance form if required

Comments: _____

Signature _____ Date _____

4. This request has been reviewed by PR for: a.) technical accuracy, b.) appropriateness for audience, c.) appropriateness of distribution statement, d.) technical sensitivity and economic sensitivity, e.) military/national critical technology, and f.) data rights and patentability

Comments: _____

APPROVED/APPROVED AS AMENDED/DISAPPROVED

LESLIE. S. PERKINS, Ph.D (Date)
Staff Scientist
Propulsion Directorate

PR2000 CHSSI Review

Computational Chemistry and Materials Science CTA

Dr. Leslie S. Perkins

CTA Leader

U.S. Air Force Research Laboratory

Propulsion Directorate

Edwards AFB, CA

CCM

Computational Chemistry and Materials Science

Distribution A: Approved for public release - distribution unlimited

CHSSI

CCM Concerns within DoD

20021122 016

- *Conductive and insulative materials for communications systems and sensors*
- *Aging and Surveillance of DoD stockpiles*
- *Contaminant decomposition within a known environment*
- *Energetic fuels and oxidizers for propulsion in critical military systems*
- *Low-observable coatings to protect the warfighter*

Project Summary

<i>Project</i>	<i>Scalability Range</i>	<i>Platforms</i>	<i>Deliverables</i>
CCM-1 : Car-Parrinello Methods for Solids	23% - 70%	Origin 2000 IBM SP	ACRES DoDPW
CCM-2: Quantum Chemistry	60% - 80%	IBM SP Cray T3E	GAMESS SAPT
CCM-3: Tight Binding Molecular Dynamics	62% - 97%	Origin 2000 IBM SP	TBLibrary Static TBMD
CCM-4: Classical Molecular Dynamics	44% - 80%	Origin 2000 Cray T3E	FMD PIMD/CMD

CCM-1: Car-Parrinello Methods for Solids

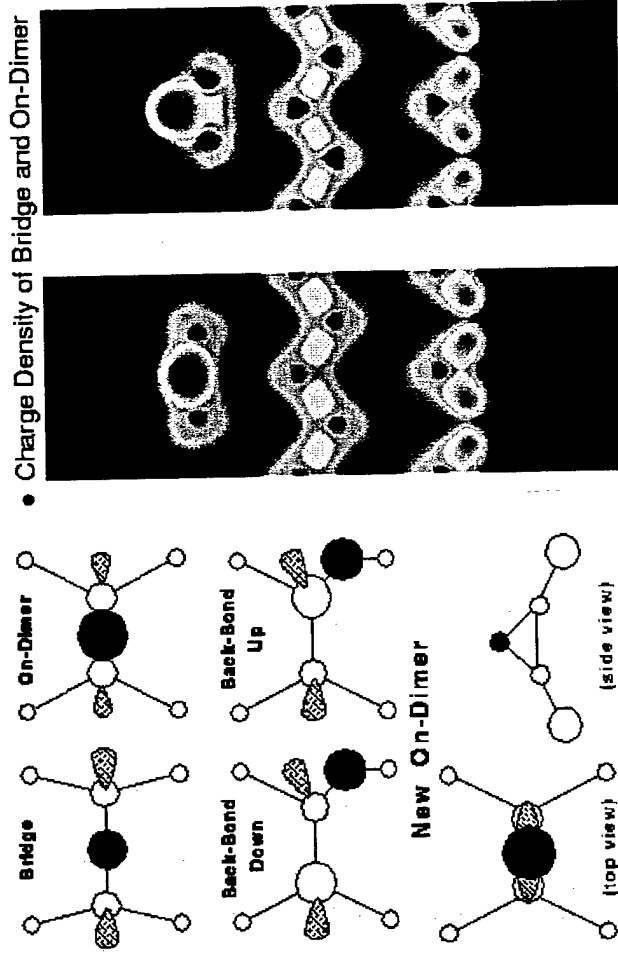
■ Synopsis

- **Objective:** Produce density functional codes (Car-Parrinello) to be used in DoD materials research
- **Partners:** Harvard, NRL
- **Development Paradigm:**
 - DoDPW: FORTRAN90, C, MPI
 - ACRES: FORTRAN90, C, HPF

■ Performance

- **Beta Testing Complete**
- **Scalability:** (32 P.E.)

	SP	O2K
DoDPW	52	31
ACRES	47	25



■ Management

- **Leveraging:** NRL, ONR (Harvard)
- **Transition Approach:** Code supported by NRL
- **Funding** \$1,672K (FY96-00)

CCM

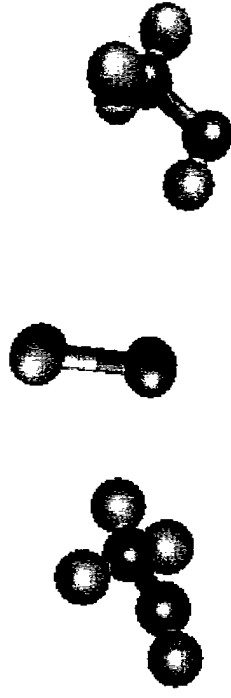
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CCM-2: Quantum Chemistry

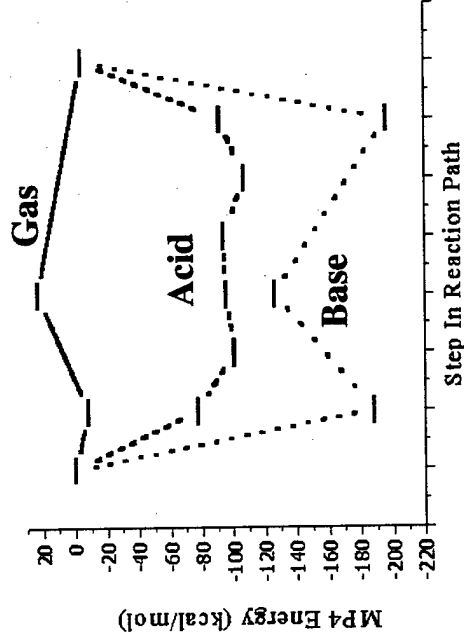
■ Synopsis

- **Objective:** Produce ab initio chemistry codes to investigate new chemical species
- **Partners:** AFRL/ML, U. of Delaware, Iowa State U.
- **Development Paradigm:** FORTRAN77, MPI



Base Catalysis - POSS synthesis

Reaction Pathways – Formation of POSS



■ Performance

- **Beta Testing Complete**
- **Scalability:** 57% (SP)
50% (O2K)
- **Operating Platforms:** SP, O2K

■ Management

- **Leveraging:** DoE, NSF
- **Transition Approach:** Used by 1,000+ users world-wide
- **Funding** \$1,593K (FY96-00)

CCM

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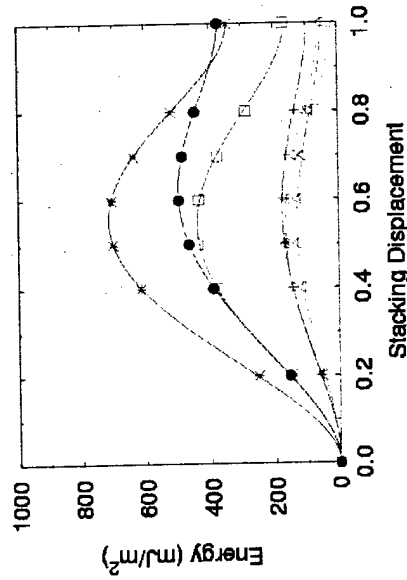
CCM-3: Tight Binding Molecular Dynamics

■ Synopsis

- **Objective:** Develop a general purpose tight-binding MD code and associated libraries
- **Partners:** *Ohio State University, George Mason University* to be consistent w/ others
- **Development Paradigm:** FORTRAN77, MPI

First Principles Calculation of Mechanical Properties:
Stacking Fault Energies and Ductility Criterion

D. A. Papaconstantopoulos and M. J. Mehl
Center for Computational Materials Science
Naval Research Laboratory
Washington DC



	Ir	Rh	Pt	Pd	Al	Pb	Cu	Au	Ag
γ_s	2590	2460	2510	1570	870	888	1730	1480	1140
γ_{111}	902	714	497	439	176	166	162	129	108
D	0.87	1.04	1.53	1.08	1.50	1.59	3.24	3.48	3.20

■ Performance

- **Beta Testing Complete**
- **Scalability:** (16 P.E.)

	SP	O2K
Fitting	-	40
Static	50	95
TBMD	62	97

■ Management

- **Leveraging:** NRL
- **Transition Approach:** Supported by NRL
- **Funding** \$1,954K (FY96-00)

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CCM-4: Classical Molecular Dynamics

■ Synopsis

- **Objective:** Develop a molecular dynamics package that can realistically simulate large molecular systems for long time scales
- **Partners:** AFRL, ARL, Iowa State U., U. of Utah, U. of Michigan, U. of Houston, Cornell U.
- **Development Paradigm:** FORTRAN77, MPI

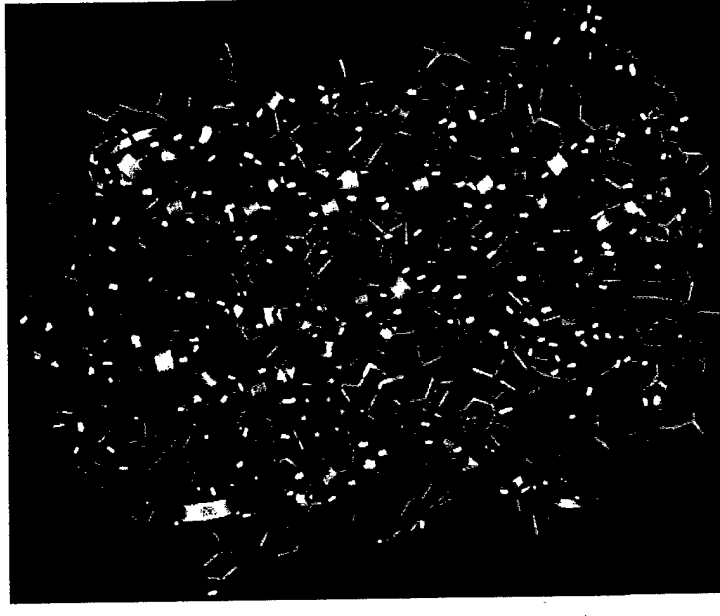
■ Performance

- **Beta Testing Complete**
- **Scalability:**

	T3E	SP	O2K
FMD	40	40	44
CMD	-	85	80

■ Management

- **Leveraging:** AFRL, AFOSR
- **Transition Approach:** Supported by AFRL
- **Funding** \$1,793K (FY96-00)



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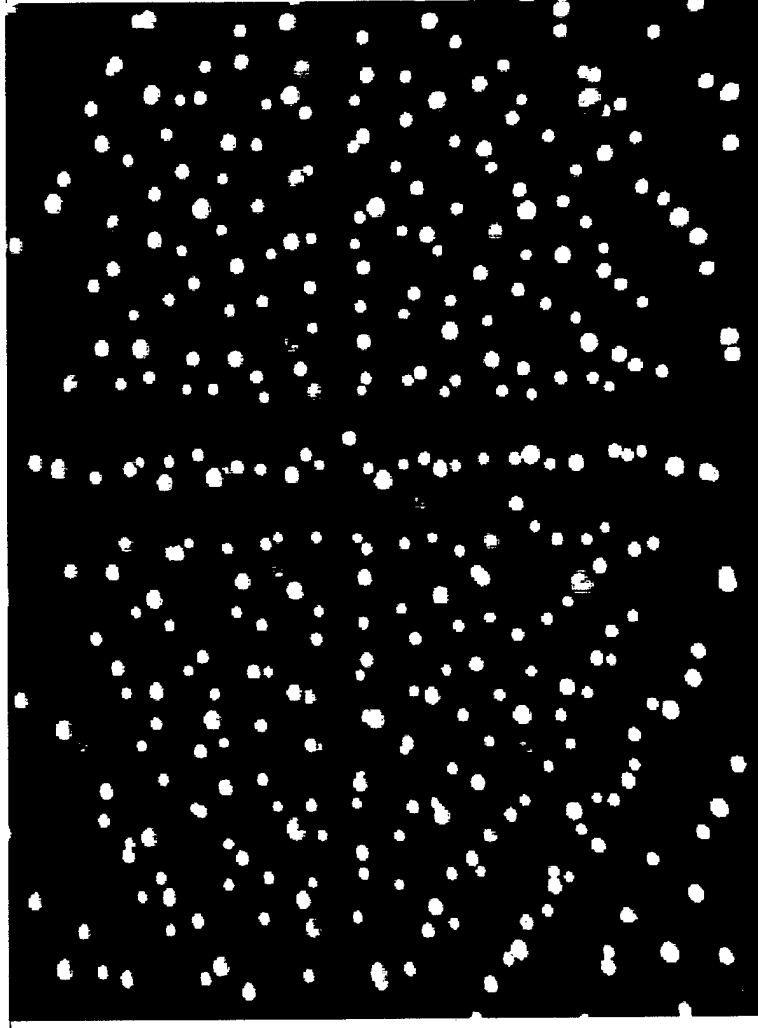
CHSSI

Applications of CHSSI Technology

■ Problem

- **Objective:** Is there global recombination of boron atoms in a solid hydrogen matrix if a single recombination is initiated?
- **Technology Used:** CMD (CCM-4)
- **Technical Team:** U. of Utah, AFRL/PR

Hydrogen ○ — are these supposed to be different?
Non-reacting Boron atom ○
Reacting Boron atom ○



■ Impact...

- **of Code Application:** The thermal conductivity of the hydrogen matrix is sufficient to prevent global recombination of boron atoms in solid hydrogen
- **of CHSSI:** This calculation would be take over ^{one}1 year, possibly two, to complete. The parallel CMD performs the calculations in ^{five}5 weeks on 64 nodes of an IBM SP.

CCM

Computational Chemistry and Materials Science

CHSSI

Applications of CHSSI Technology

■ Problem

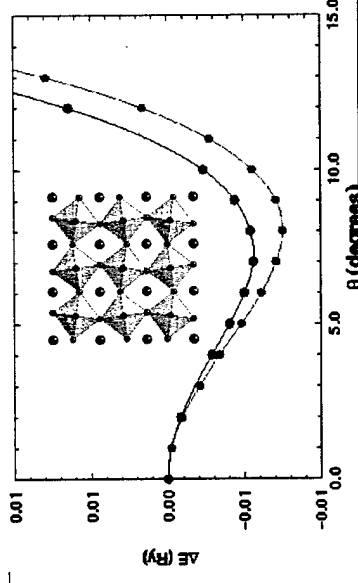
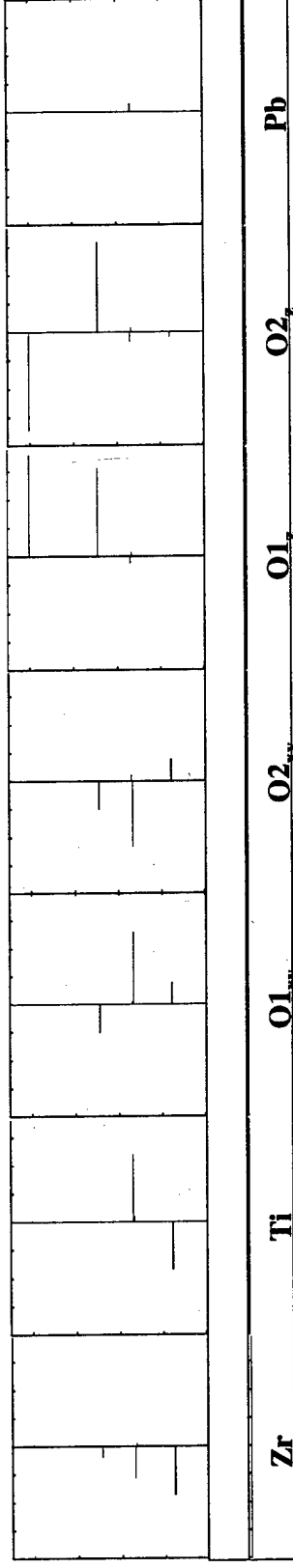
- **Objective:** Determine if Pb can be removed from PZT [Pb(Zr,Ti)O₃] a Navy Sonar Material, and maintain its effectiveness

• **Technology Used:** DoDPW, NRL-LAPW

• **Technical Team:** NRL, ONR

Phonon displacement patterns and frequencies in PZT 50-50 supercell

800
600
400
200
0
200 i



Rotational Instability in Ferroelectric PZT 50-50 supercell.

■ Impact...

- **of Code Application:** ONR and NRL are gaining a crucial understanding of how the Pb effects the sonar material
- **of CHSSI:** The code accurately describes the material and researchers will be able to suggest effective substitutes within a short time

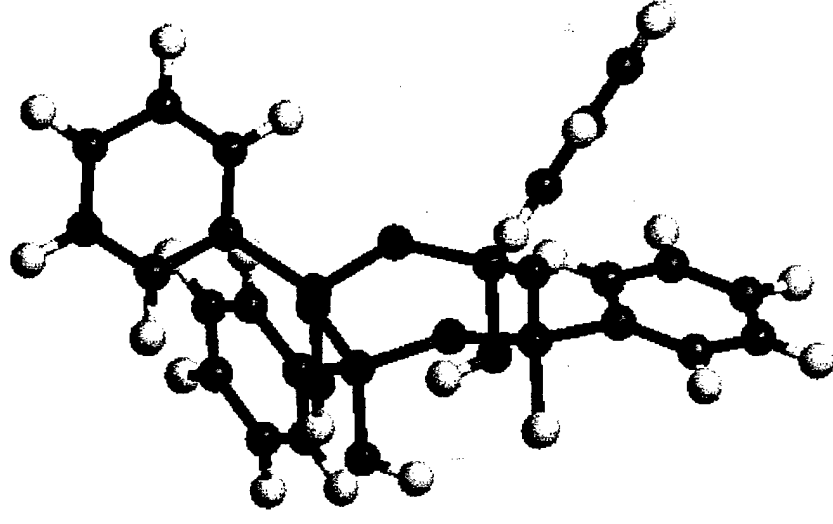
CCM
Computational Chemistry and Materials Science

CHSSI

Applications of CHSSI Technology

■ Problem

- **Objective:** Identify important factors in the synthesis of polyhedral oligomeric silsesquioxanes (POSS) to modify the existing lengthy synthesis process
- **Technology Used:** GAMESS (CCM-2)
- **Technical Team:** AFRL, Iowa State U., ASC MSRC PET



■ Impact...

- **of Code Application:** The effects of solvents led to a new process for the formulation of POSS. of different catalysts and solvents have been found to be crucial in the quick formulation of POSS.
- **of CHSSI:** The calculation to determine the structure and associated energies lasted approximately 1st week. The serial version would require over ONE YEAR of dedicated time.

CCM

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CHSSI